Chenguang Wang

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Education

•The Chinese University of Hong Kong, Shenzhen *2022.09-Present*
PhD in Computer Science Supervisor: Tianshu Yu

•University of Chinese Academy of Sciences *2019.09-2022.06*
Master of Science, Operations Research and Cybernetics Supervisor: Tiande Guo

•Zhengzhou University *2015.09-2019.06*
Bachelor of Science, Mathematics and Applied Mathematics

Research Interests

- **Learning to Optimize:** Efficient training algorithms, improve generalization ability
- **Diffusion Based Sampling (Ongoing):** Efficient sampling algorithms, distribution coverage optimization, probabilistic inference acceleration
- **Diffusion Based Generation (Ongoing):** Multimodal generation, graph structure generation, guided generation control, conditional generation optimization
- **Diffusion Based LLM (To Be Explored):** Diffusion model based large language models, generation quality enhancement, controllable text generation

Academic Achievements

Google Scholar Profile: https://scholar.google.com/citations?user=Ptf3uO0AAAAJ&hl=zh-CN

- **Published Papers:**
  - **Wang C***, Cui K*, Zhao W, et al. Sampling from Binary Quadratic Distributions via Stochastic Localization. *Proceedings of the 42nd International Conference on Machine Learning (ICML)*, 2025. **(CCF A-class)**
  - Zhao W, **Wang C**, Wang X, et al. Understanding Oversmoothing in Diffusion-Based GNNs From the Perspective of Operator Semigroup Theory. *Proceedings of the 31st ACM SIGKDD Conference on Knowledge Discovery and Data Mining (KDD)*, 2025: 2043-2054. **(CCF A-class)**
  - **Wang C**, Yu Z, McAleer S, et al. ASP: Learn a Universal Neural Solver! *IEEE Transactions on Pattern Analysis and Machine Intelligence (TPAMI)*, 2024. **(CCF A-class)**
  - **Wang C**, Fu Z H, Lu P, et al. Efficient Training of Multi-task Neural Solver for Combinatorial Optimization. *Transactions on Machine Learning Research (TMLR)*, 2025.
  - **Wang C**, Han C, Guo T, et al. Solving uncapacitated P-Median problem with reinforcement learning assisted by graph attention networks. *Applied Intelligence*, 2023, 53(2): 2010-2025.
  - Liu Z*, **Wang C***, Han C, et al. Learning Graph Representation by Aggregating Subgraphs via Mutual Information Maximization. *Neurocomputing*, 2023: 126392.
- **Preprint Papers:**
  - **Wang C**, Zhang X, Cui K, et al. Importance Weighted Score Matching for Diffusion Samplers with Enhanced Mode Coverage. *arXiv preprint* arXiv:2505.19431, 2025.
  - Pan X*, **Wang C***, Ying C, et al. Rethinking the "Heatmap+ Monte Carlo Tree Search" Paradigm for Solving Large Scale TSP. *arXiv preprint* arXiv:2411.09238, 2024.
  - **Wang C**, Pan X, Yu T. Towards Principled Task Grouping for Multi-Task Learning. *arXiv preprint* arXiv:2402.15328, 2024.
  - **Wang C**, Yang Y, Slumbers O, et al. A game-theoretic approach for improving generalization ability of TSP solvers. *arXiv preprint* arXiv:2110.15105, 2021.

Research Projects

- **Diffusion Process-based Sampling Methods** *Representative Works: ICML 2025, arXiv 2025*
  - Proposed efficient discrete sampling algorithms based on stochastic localization, achieving consistent performance improvements across multiple standard sampling benchmarks, providing new sampling frameworks for complex discrete distributions
  - Designed Neural Samplers based on Diffusion Models, effectively addressing distribution fitting bias issues through Importance Sampling, achieving SOTA effects in high-dimensional probabilistic distribution sampling tasks
  - Technical Skills: Diffusion Model theory and algorithms, MCMC-based sampling methods, high-performance PyTorch/JAX implementation
- **Combinatorial Optimization and Neural Solvers** *Representative Works: IEEE TPAMI 2024, TMLR 2025*
  - Proposed ASP universal neural routing optimization framework, integrating game-theoretic self-play mechanisms with deep reinforcement learning, constructing progressive Curriculum Learning mechanisms to overcome distribution shift and scale generalization bottlenecks
  - Designed Multi-armed Bandits-based task selection strategies to solve negative transfer problems in multi-task combinatorial optimization, achieving efficient joint training across problem types with significantly enhanced training efficiency and generalization
  - Technical Skills: Reinforcement learning, game-theoretic adversarial training, Bandit algorithms, Multi-task Learning, high-performance PyTorch implementation
- **Graph-based Deep Learning** *Representative Works: KDD 2025, Neurocomputing 2023*
  - Analyzed oversmoothing phenomena in diffusion-based continuous GNNs from operator semigroup theory perspective, proposing theoretical solutions to provide new mathematical foundations for continuous graph neural network design
  - Constructed graph representation learning framework based on mutual information maximization, significantly improving graph data representation quality through subgraph aggregation strategies
  - Technical Skills: Spectral graph analysis, graph neural networks, PyTorch Geometric implementation

Internship Experience

- **Shanghai Artificial Intelligence Laboratory**

  Research Intern 2025.07-Present
  - Designed and implemented Flow Matching-based chemical retrosynthesis generation algorithms, optimizing molecular representation learning and validating algorithm effectiveness on large-scale datasets
  - Participated in constructing end-to-end retrosynthesis prediction systems, integrating single-step retrosynthesis models with large language models to support efficient multi-step retrosynthesis inference
- **Peking University & King's College London**

  Research Intern 2021.11-2022.06
  - Applied reinforcement learning, multi-agent learning, and game theory methods to combinatorial optimization problem-solving algorithm research, proposing game-theory-based TSP solver generalization capability enhancement solutions
  - Completed research paper: A Game-Theoretic Approach for Improving Generalization Ability of TSP Solvers **(ICLR 2022 Workshop Spotlight Presentation)**
- **CAS Key Laboratory of Big Data Mining and Knowledge Management**

  Undergraduate Research Assistant 2019.03-2019.06
  - Participated in generative adversarial network-related theoretical research, completing comprehensive survey and analysis of GAN technologies
  - Completed undergraduate thesis "A Comprehensive Survey on Generative Adversarial Networks" **(Outstanding Thesis, Zhengzhou University)**

Honors and Awards

- Shenzhen Institute of Big Data PhD Student Scholarship (2023-2025)
- ICLR 2022 Workshop on Gamification and Multiagent Solutions Spotlight Presentation
- Outstanding Participant in Oxford International Exchange Program
- Outstanding Undergraduate Thesis Award: "A Comprehensive Survey on Generative Adversarial Networks"